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## SIMULATING THE DYNAMICS OF PARTICLES INTERACTING WITH SOLIDIFICATION FRONTS (PREPRINT - BRIEFING CHARTS)

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### CONFERENCE PAPER PREPRINT (BRIEFING CHARTS)

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# Simulating the Dynamics of Particles Interacting with Solidification Fronts

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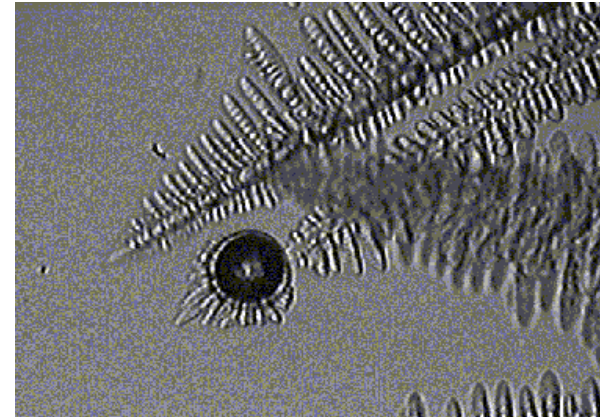
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# Motivation

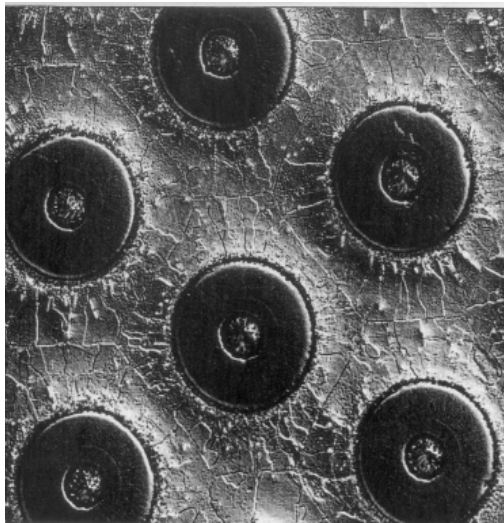
- Particle-solidification front interactions play a crucial role in predicting microstructures of metal-matrix composites (MMCs)



MMCs: Micron-sized particles embedded in a metal matrix – acts as reinforcement

Industries: Automotive, aerospace

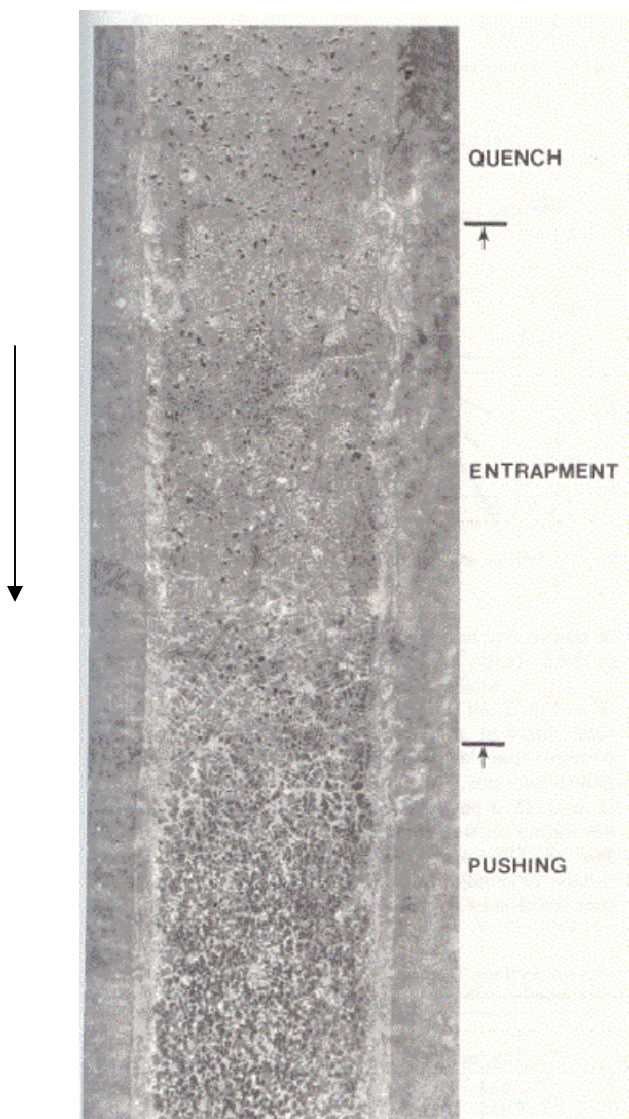
Properties: lightweight, good wear resistance



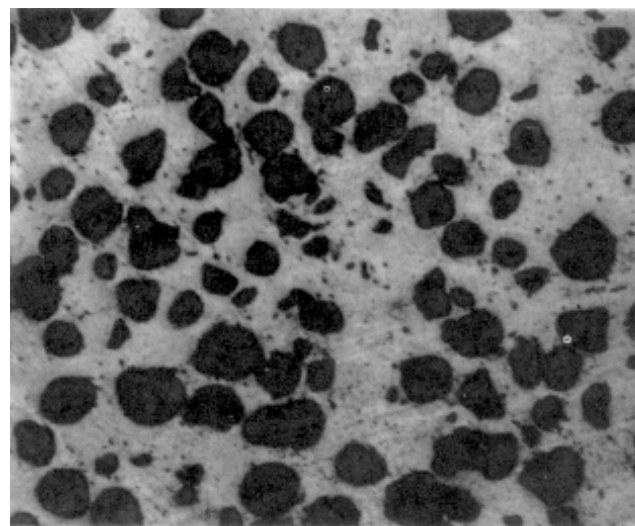


# Processing of MMCs

Directionally solidified Al-17Cu/SiC. 21x



As-cast Al-2Mg/20 wt pct graphite. 31x



Want: Uniform distribution of particles  
Need: Understand particle-front interactions

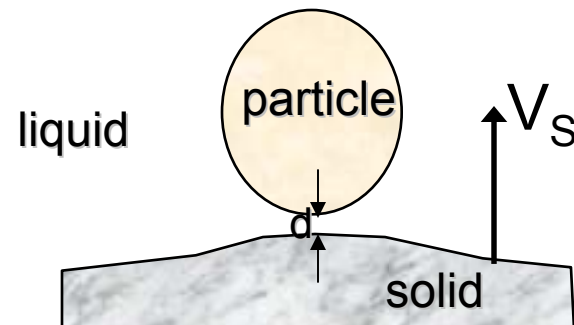




# What happens when a solidification front interacts with a particle?



- As solidifying front approaches a particle it will either be
  - Engulfed
  - Pushed
  - Pushed, then engulfed



- Critical velocity,  $V_{CR}$ 
  - Solidification velocity,  $V_s \leq V_{CR} \rightarrow$  particle pushing
  - $V_s > V_{CR} \rightarrow$  particle engulfment

◆ **Challenge:** A multiscale model that couples the dynamics in the gap with the overall thermal/fluid transport



# Physics of particle-solidification front interactions

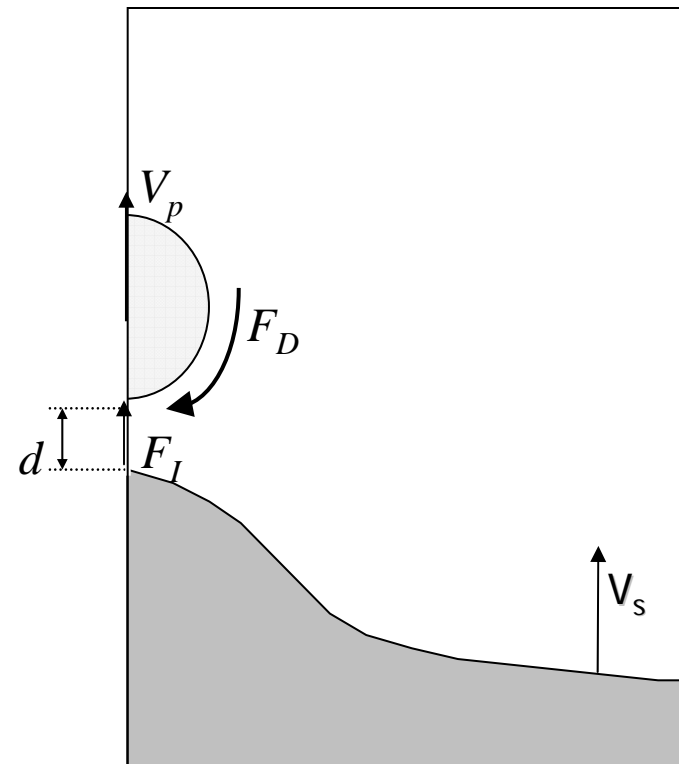


## Dynamics of the particle

- Force balance on the particle

$$m_p \frac{dV_p}{dt} = F_I - F_D$$

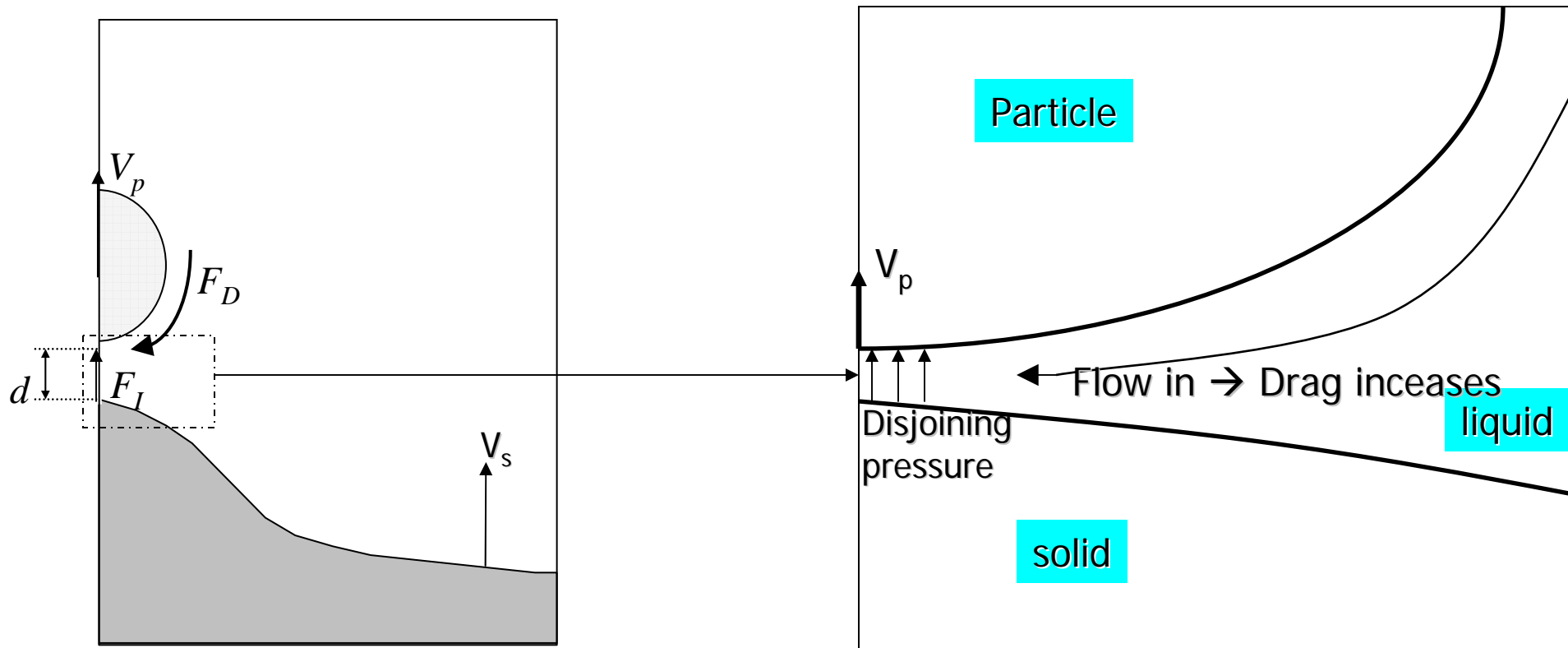
- $F_I$  is the repulsive interaction force
- $F_D$  is an attractive drag force
- Balance determines whether the particle will be engulfed/pushed







# Fluid mechanics and thermal transport

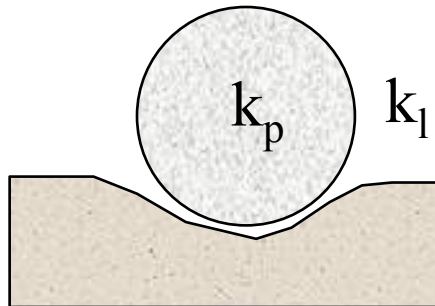


- In addition, thermal conditions affect the critical velocity. Large scale effects (thermal conductivity differences between the particle and the solidification front), and small scale effects (premelting film).



## The thermal conductivity issue

- ◆  $k_p/k_l$  has a significant impact on whether a particle is pushed/engulfed



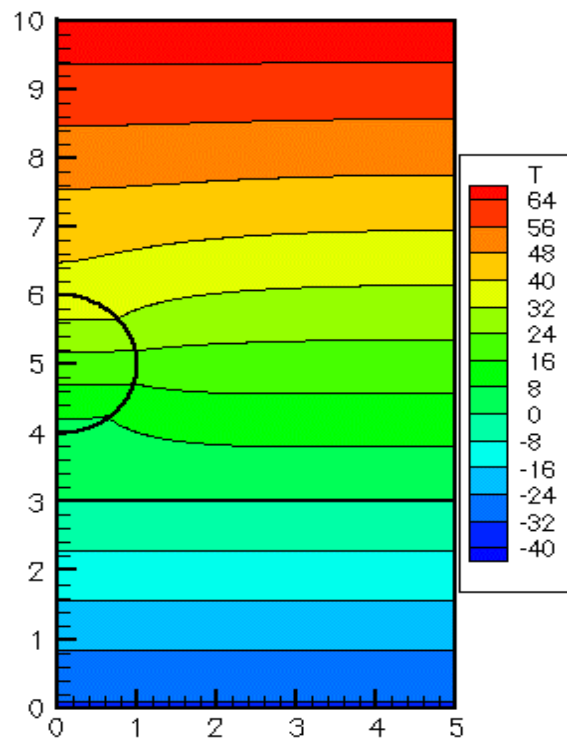
- ◆ In fact, experimental observations have shown that:
  - ◆ Engulfment 100% of the time for  $k_p/k_l > 1.0$
  - ◆ Pushing for  $k_p/k_l < 1.0$
- ◆ Why does the  $k_p/k_l$  have such a significant impact?



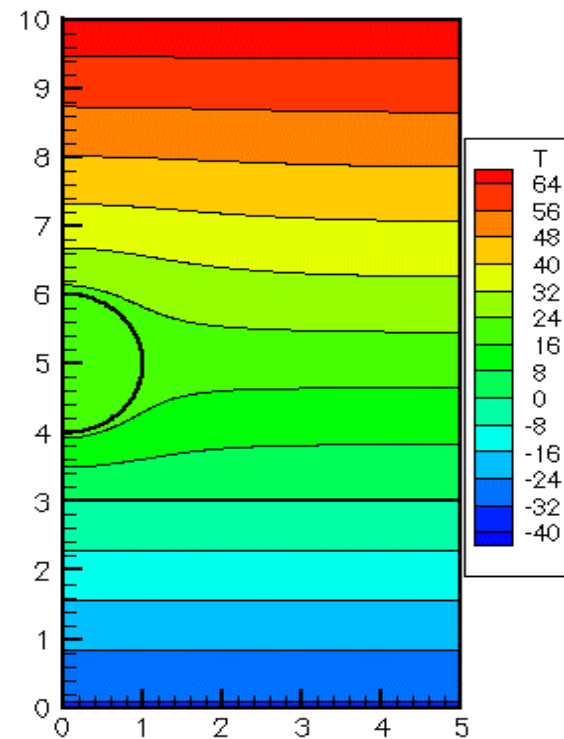
# How does the $k_p/k_l$ influence the interface shape?



$$k_p/k_l < 1.0$$



$$k_p/k_l > 1.0$$





Summary: The thermal conductivity ratio,  $k_p/k_l$ , has a significant impact on whether a particle is pushed/engulfed → this is a micro-scale phenomenon (scale of the particle)

What about nano-scale phenomena?



## Premelted films

$$T < T_m$$



Film thickness: 
$$d = \left( -2\sigma^2 \frac{\Delta\gamma}{\rho_l \Delta H_f} \right)^{1/3} t^{-1/3}$$

Atomic radius:  $\sigma$

Liquid density:  $\rho_l$

Latent heat per molecule:  $\Delta H_f$

$$t = \frac{T_m - T_i}{T_m}$$

$$\Delta\gamma = \gamma_{sp} - (\gamma_{lp} + \gamma_{ls})$$



# Premelting film theory effect on interface temperature of a solidification front



$$T_i = T_m - \left( \frac{\lambda}{d} \right)^{\nu} T_m$$

$T_i$  is the interface temperature

$T_m$  is the melting temperature

$\nu = 3$  for van der Waals

$\lambda$  is an interaction length scale (nanometer scale)



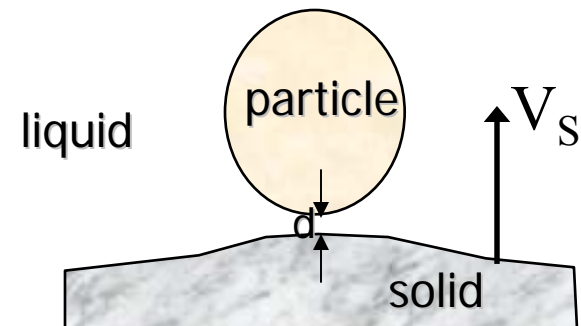
## Disjoining pressure theory

- Disjoining pressure  $\longrightarrow \Pi = \frac{A}{6\pi d^3}$ 
  - Nano-scale force
  - Molecular in nature

$A = \text{Hamaker constant} \sim \Delta\gamma$

$\Delta\gamma = \gamma_{sp} - (\gamma_{lp} + \gamma_{ls}) \longrightarrow \begin{array}{l} \Delta\gamma > 0 \rightarrow \text{repulsive} \\ \Delta\gamma < 0 \rightarrow \text{attractive} \end{array}$

- Van der Waals?







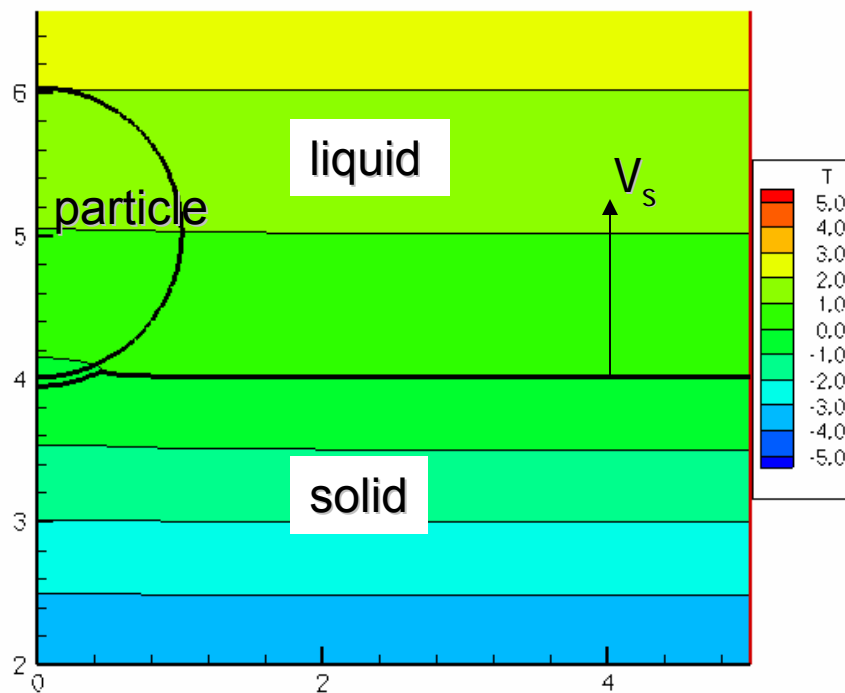
Previous work on thermal effects of premelted layers on particle-  
solidification front dynamics  
(Garvin and Udaykumar, Journal of Crystal Growth (2005))



# Premelting film theory effect on interface temperature of a solidification front

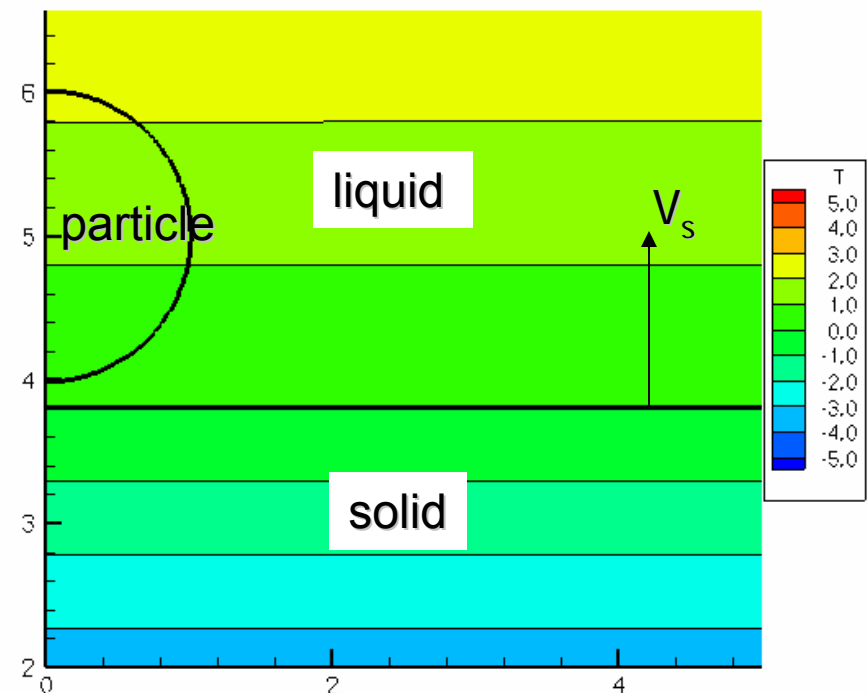


V<sub>pull</sub> = 1000 microns/sec - includes premelting effects



$$T_i = T_m - \left( \frac{\lambda}{d} \right)^v T_m$$

V<sub>pull</sub> = 1000 microns/sec - No premelting effects

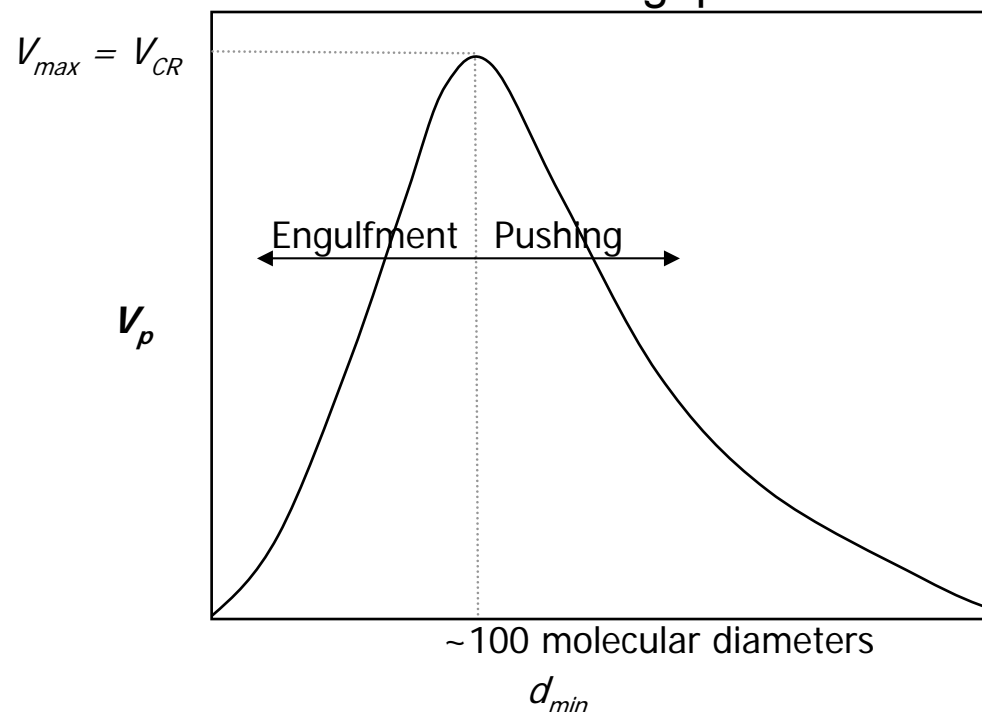


$$T_i = T_m$$



## The premelting effect on $V_{CR}$

- 2 approaches when modeling
  - 1) Not to include premelting in the interaction
    - Requires setting a gap thickness cut-off value for engulfment (ad hoc)
  - 2) Including premelting (Rempel and Worster)
    - Linear stability analysis, steady-state and  $k_p/k_l = 1.0$
    - No need for ad-hoc cut-off for gap thickness





## Summary of physics

- $k_p/k_l$  ratio greatly affects the critical velocity (micro-scale effect)
  - Alters the interface shape
    - $k_p/k_l < 1.0$ , bump forms that promotes pushing
    - $k_p/k_l > 1.0$ , trough forms that promotes engulfing (higher drag)
- Premelting film
  - Liquid layer wants to exist between the front and the particle
    - Also alters interface shape
    - If no premelting is assumed, gap thickness cut-off value is needed

The  $k_p/k_l$  effects act on a larger (microscale) whereas the premelting/disjoining pressure effects act on a “nano”-scale



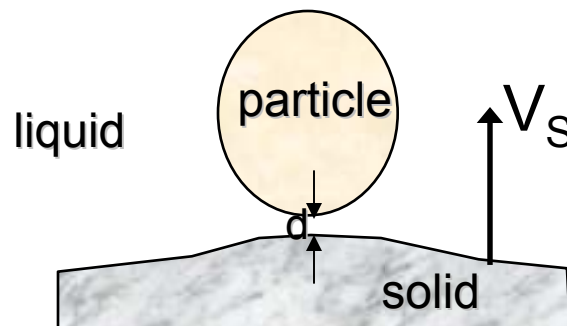
PROBLEM: How to model particle-solidification  
front interactions?



## In the past ...

- Theoretical research relied on...
  - 1) All-simplified models for the forces acting on the particle
  - 2) All-qualitative explanations/models based off of thermal property considerations
  - 3) Most on steady-state analysis
  - 4) Most- Do not assume a premelting layer in the gap
  - 5) All-assumed stable (non-dendritic solidifications front)

ALL MODELS ATTEMPT TO FIND CRITICAL VELOCITY





## OUR APPROACH...

Lubrication Model for the flow in the gap between the front and particle and NS for outer flow – match solutions (matched numerics)





# Advantages

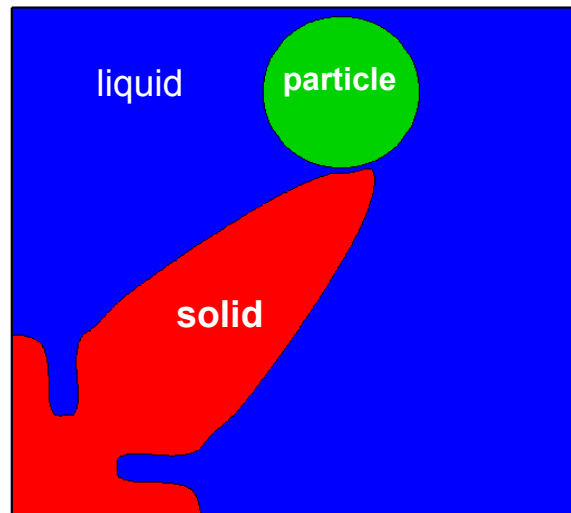
1. Capture dynamics (i.e. not a steady-state solution)
2. Premelting effects will be included
3.  $k_p/k_l$  effects will be captured from the governing equation
4. Do not have to rely on simple force models as the lubrication equation will contain a repulsive body force
5. Can be generalized for a variety of problems involving solid body interactions (including dendrite+particle)



# Modeling of particle-front interactions

## Main Ingredients:

1. Solidification front and the particle are tracked using a sharp-interface level-set method with transport variables solved via NS equations “outer region”
2. Solution in the gap is treated as a lubrication layer, so a different set of equations are needed “inner region”
3. The solution of the “inner” and “outer” regions are coupled through BCs.  
“matching region”





## Outer transport equations

- Navier-Stokes Equations (with mass and energy conservation):

Continuity equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

x-Momentum equation:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\mu}{\rho} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

y-Momentum equation:

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{\mu}{\rho} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)$$

Energy equation:

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \alpha_{s/l/p} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

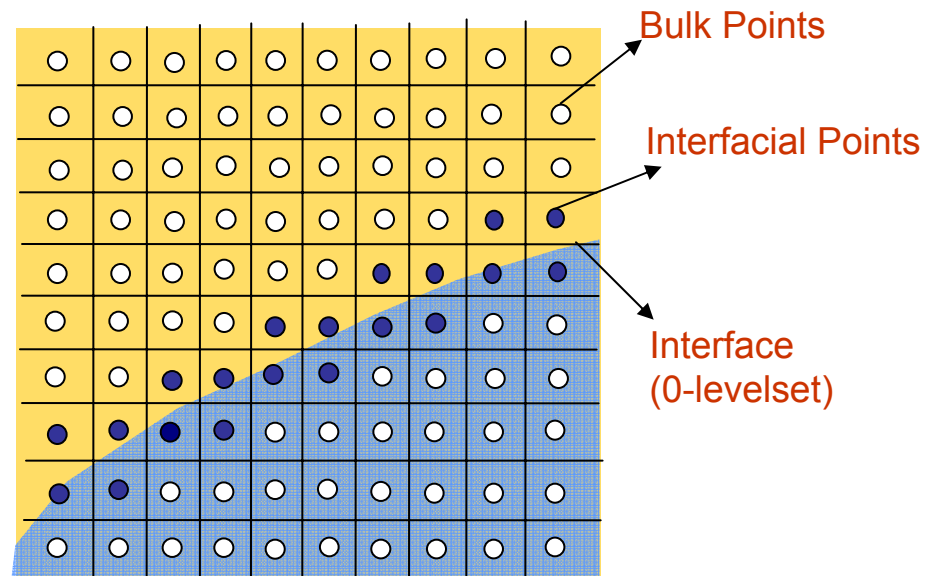
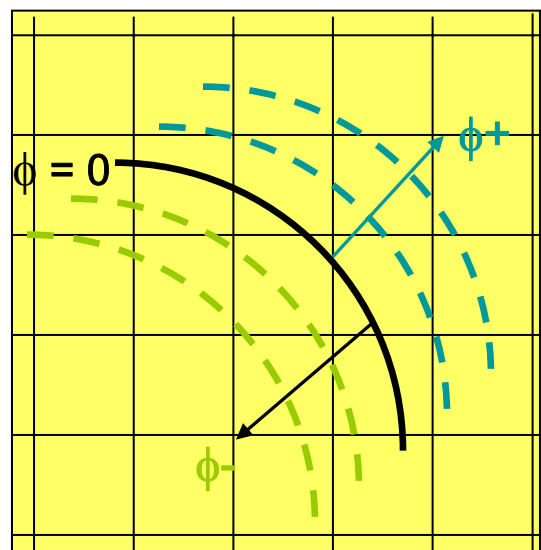
Interface conditions:

$$\rho H_{sk} \dot{V}_{N'} = k_s \left. \frac{\partial T}{\partial n} \right|_s - k_l \left. \frac{\partial T}{\partial n} \right|_l$$



# Level-Set Method

Level-set function ( $\phi$ ) - Signed normal distance from the interface



$$\phi_t + \vec{V} \cdot \vec{\nabla} \phi = 0$$

Level-set Advection

$$\vec{N} = \vec{\nabla} \phi / |\vec{\nabla} \phi|$$

Normal

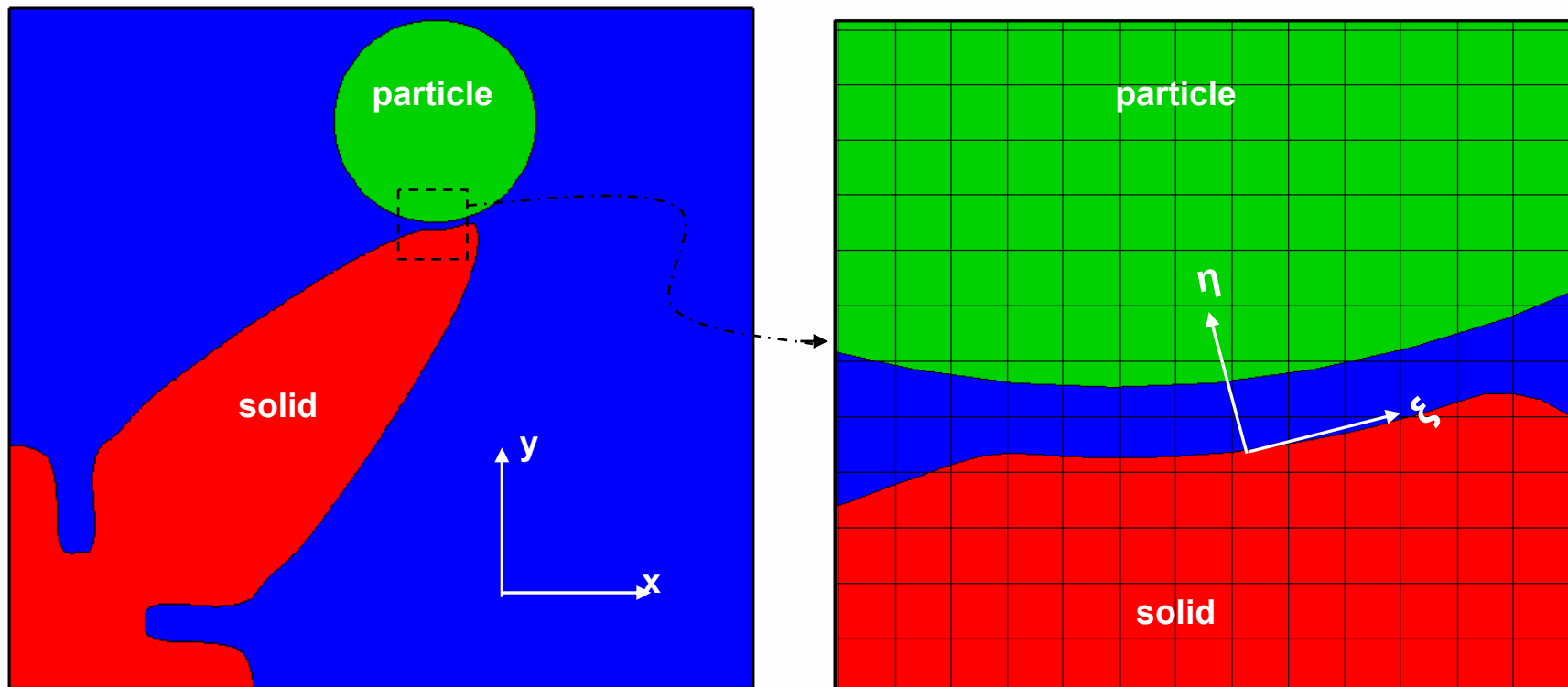
$$\kappa = -\vec{\nabla} \cdot \vec{N}$$

Curvature



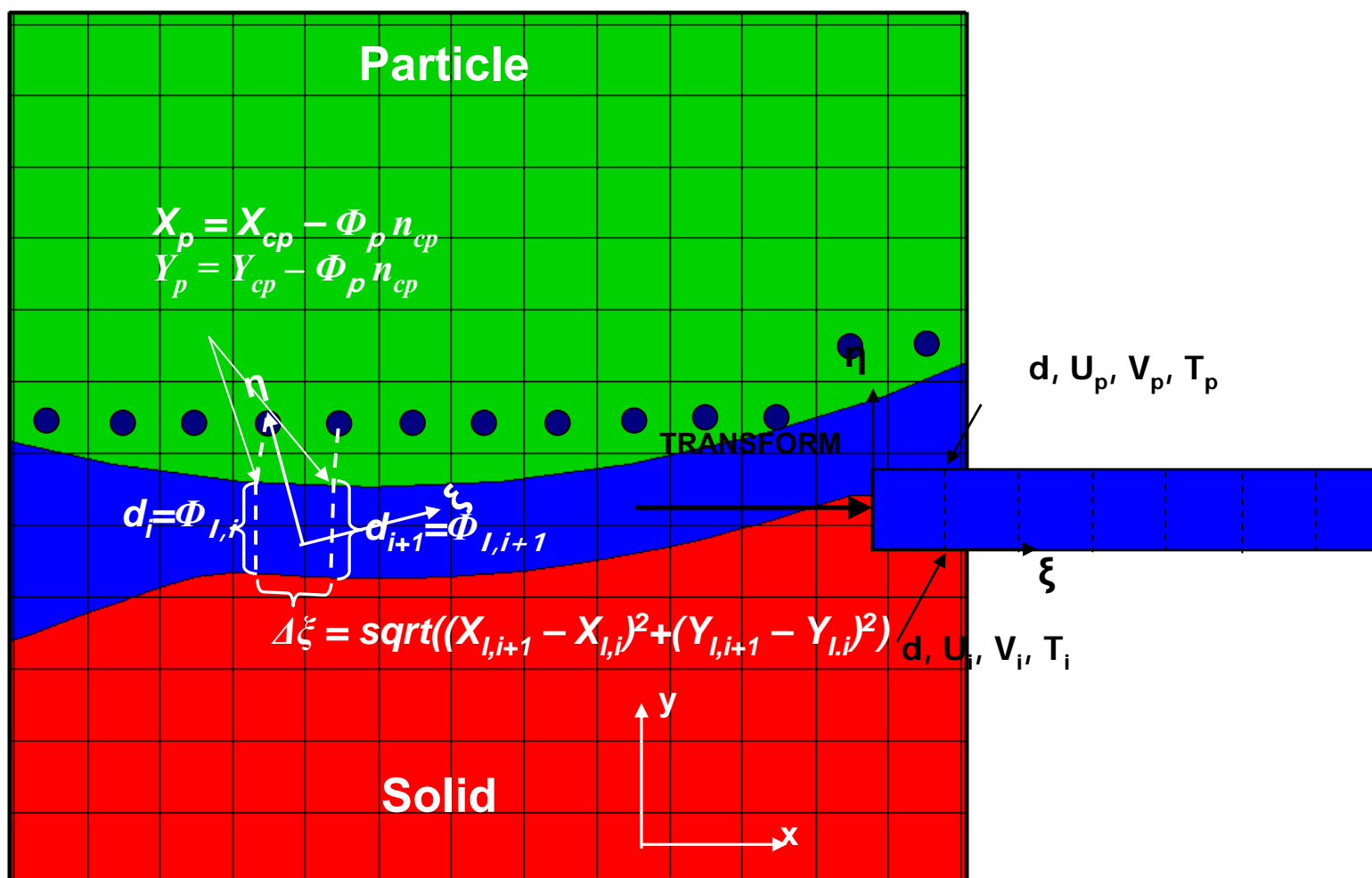
## Using a Lubrication Model for “inner” region

- Lubrication Model
  - One direction of the fluid flow and the heat flow is assumed to have negligible effects compared to other directions
  - The need for a mesh in one direction is eliminated
    - Interaction in the gap (disjoining pressure included) can be accounted for in lubrication model





## Using a Lubrication Model for “inner” region





## Transformed NS equations from $x,y \rightarrow \xi,\eta$

Continuity:

$$\frac{\partial U}{\partial \xi} + \frac{\partial V}{\partial \eta} = 0$$

u-momentum (v-momentum and Energy equation are very similar):

$$\frac{\partial(J\rho u)}{\partial t} + \frac{\partial(\rho U u)}{\partial \xi} + \frac{\partial(\rho V u)}{\partial \eta} = -\left\{ \frac{\partial y}{\partial \eta} \frac{\partial p}{\partial \xi} - \frac{\partial y}{\partial \xi} \frac{\partial p}{\partial \eta} \right\} + \frac{\partial}{\partial \xi} \left[ \frac{\mu}{J} \left( q_1 \frac{\partial u}{\partial \xi} - q_2 \frac{\partial u}{\partial \eta} \right) \right] + \frac{\partial}{\partial \eta} \left[ \frac{\mu}{J} \left( q_3 \frac{\partial u}{\partial \eta} - q_2 \frac{\partial u}{\partial \xi} \right) \right] - \underbrace{\left\{ \frac{\partial y}{\partial \eta} \frac{\partial \Pi}{\partial \xi} - \frac{\partial y}{\partial \xi} \frac{\partial \Pi}{\partial \eta} \right\}}_{\substack{\text{Disjoining} \\ \text{Pressure} \\ \text{terms treated} \\ \text{as body force}}}$$

Where:  $u,v \rightarrow x,y$  velocities;  
 $U,V \rightarrow \xi, \eta$  velocities,





## Orthogonal coordinates ( $q_2=0$ ) and do scaling analysis

Scaling:  $\xi^* = \frac{\xi}{L} \quad \eta^* = \frac{\eta}{d}$

By assuming small curvatures in the interfaces and using the fact that:

$$U = uy_\eta - vx_\eta \quad V = vx_\eta - uy_\xi$$

To get:

Mass:  $\frac{\partial U^*}{\partial \xi^*} + \frac{\partial V^*}{\partial \eta^*} = 0$

U-mom:  $-\left(\frac{(J^*)^3}{J_{No}^* q_3^*}\right) \left(\frac{\partial p^*}{\partial \xi^*} + \frac{\partial \Pi^*}{\partial \xi^*}\right) + \frac{\partial^2 U^*}{\partial \eta^{*2}} = 0$

V-mom:  $\left(\frac{\partial p^*}{\partial \eta^*} + \frac{\partial \Pi^*}{\partial \eta^*}\right) = 0$

Energy:  $\frac{\partial^2 T^*}{\partial \eta^{*2}} = 0$

Notice that  $p^*$  and  $\Pi^*$  only depend on  $\xi^*$



## Pressure Equation in the gap

$$-\left(\frac{(J)^3}{J_{NO}q_3}\right)\left[\left(\frac{\partial^2 p}{\partial \xi^2} + \frac{\partial^2 \Pi}{\partial \xi^2}\right)\frac{d^3}{12} + \left(\frac{\partial p}{\partial \xi} + \frac{\partial \Pi}{\partial \xi}\right)\frac{\partial d}{\partial \xi}\left(\frac{d^2}{4}\right)\right] + \frac{1}{2}\left(d\frac{\partial(U_p - U_i)}{\partial \xi} + (U_p - U_i)d^2\frac{\partial}{\partial \xi}\left(\frac{1}{d}\right)\right) + V_p - V_i = 0$$

BCs: At  $\xi=0$ ,  $p=p_{\text{outer},0}$   
At  $\xi=L$ ,  $p=p_{\text{outer},L}$

Temperature Equation:  $T = \left(\frac{T_p - T_i}{d}\right)\eta + T_i$



# Coupling the outer flow equations to the inner lubrication equations

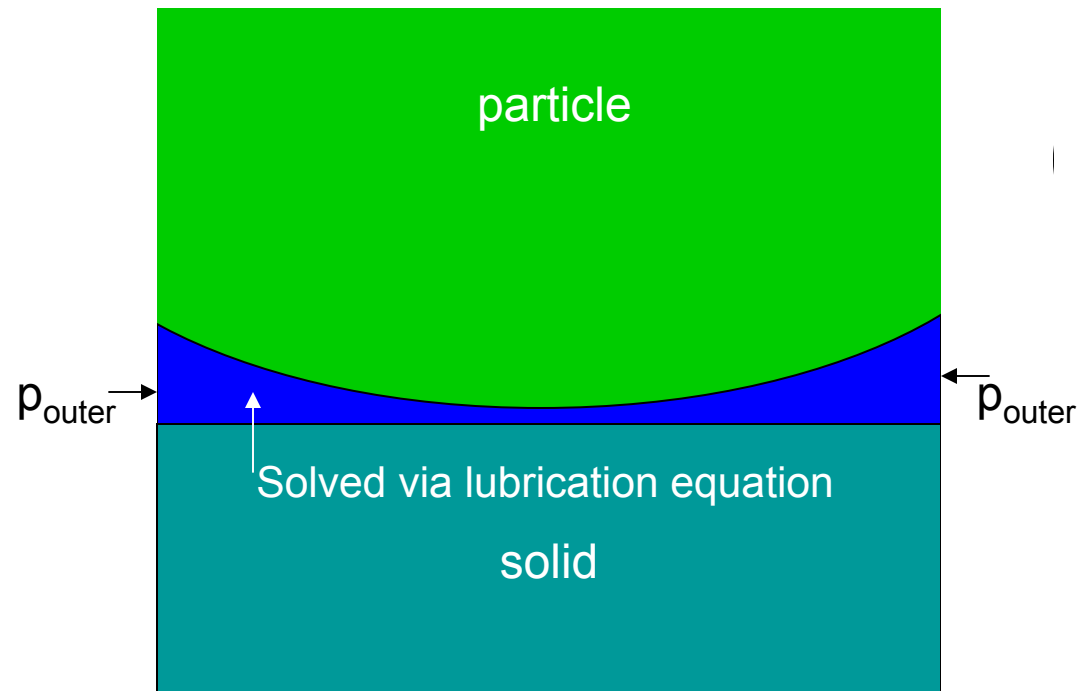
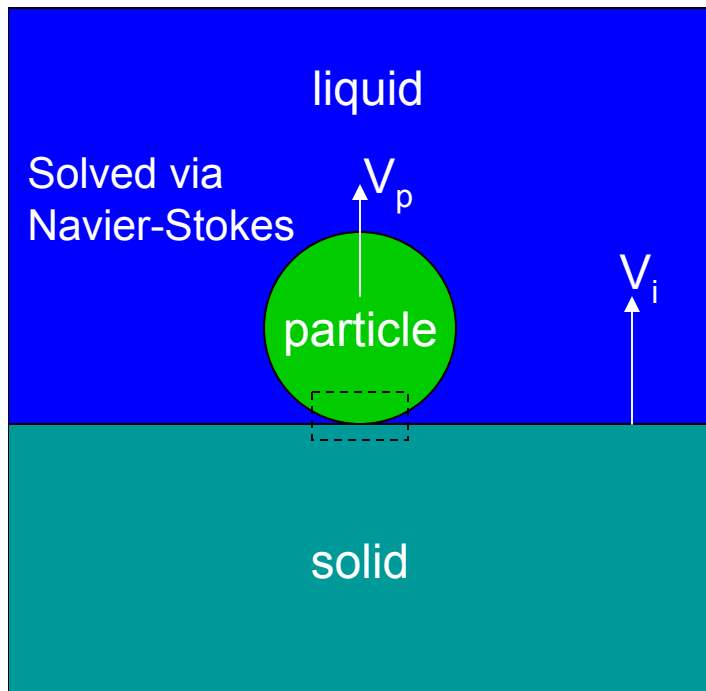


# How are the Boundary conditions applied to the lubrication model?



BCs:            At  $\xi=0$ ,  $p=p_{\text{outer}}$   
                     At  $\xi=L$ ,  $p=p_{\text{outer}}$

Edge of the lubrication layer is 8 mesh pts.  $\rightarrow$  enough resolution for outer flow

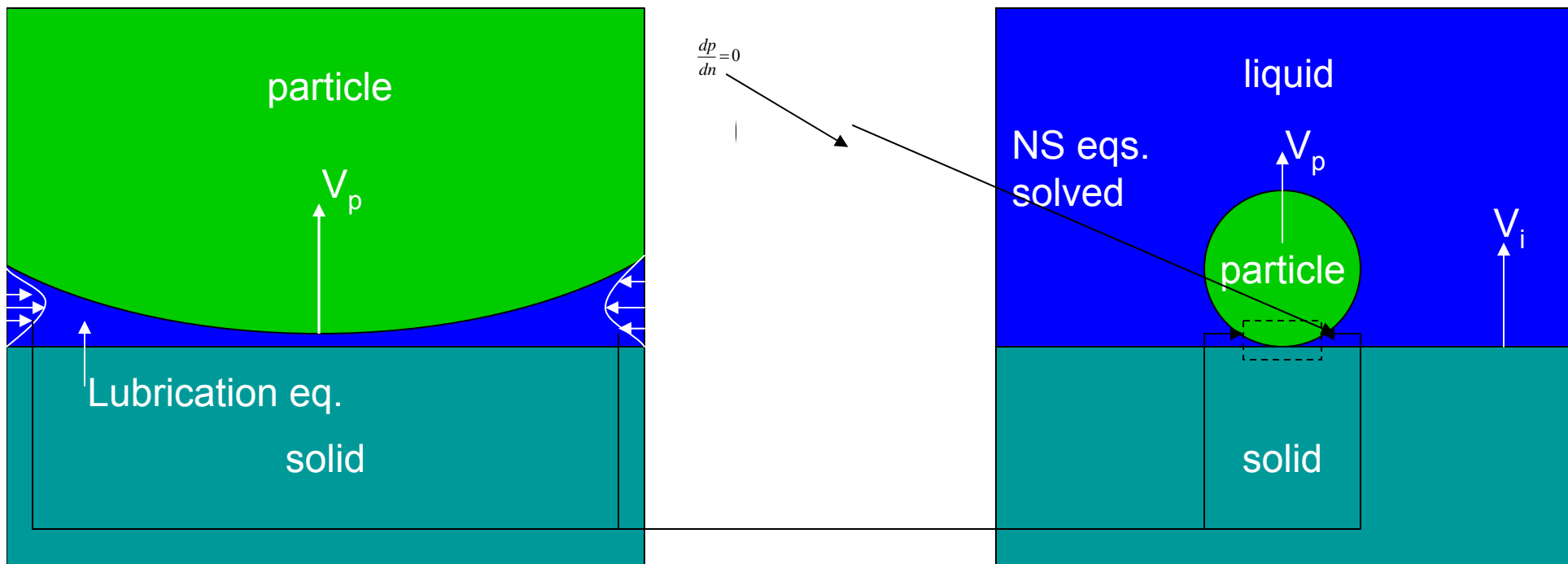




# How are the Boundary conditions applied to the outer flow (solved via NS)?



BCs: at the edges of lubrication layer, find a parabolic velocity profile that satisfies mass conservation (treated as outlets)





## Forces acting on the bodies

The forces acting on the bodies can now be obtained from the outside flow and the inner lubrication flow, so:

$$\sum \vec{F} = \vec{F}_{INNER} + \vec{F}_{OUTER}$$

$$\vec{F}_{INNER} = - \int_A p_{INNER} d\vec{S}$$

$$\vec{F}_{OUTER} = - \int_A p_{OUTER} d\vec{S}$$



## The temperature of the interfaces?

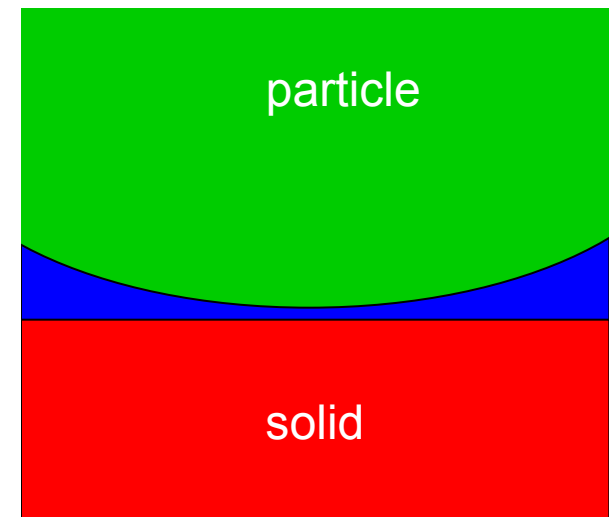
Temperature of the solidification front is found via:

$$T_i = T_m - \left( \frac{\lambda}{d} \right)^v T_m \longrightarrow \text{premelting}$$

$$T_i = T_m \longrightarrow \text{No premelting}$$

The d-distribution is found from the level set information  
The particle interface temperature is found from:

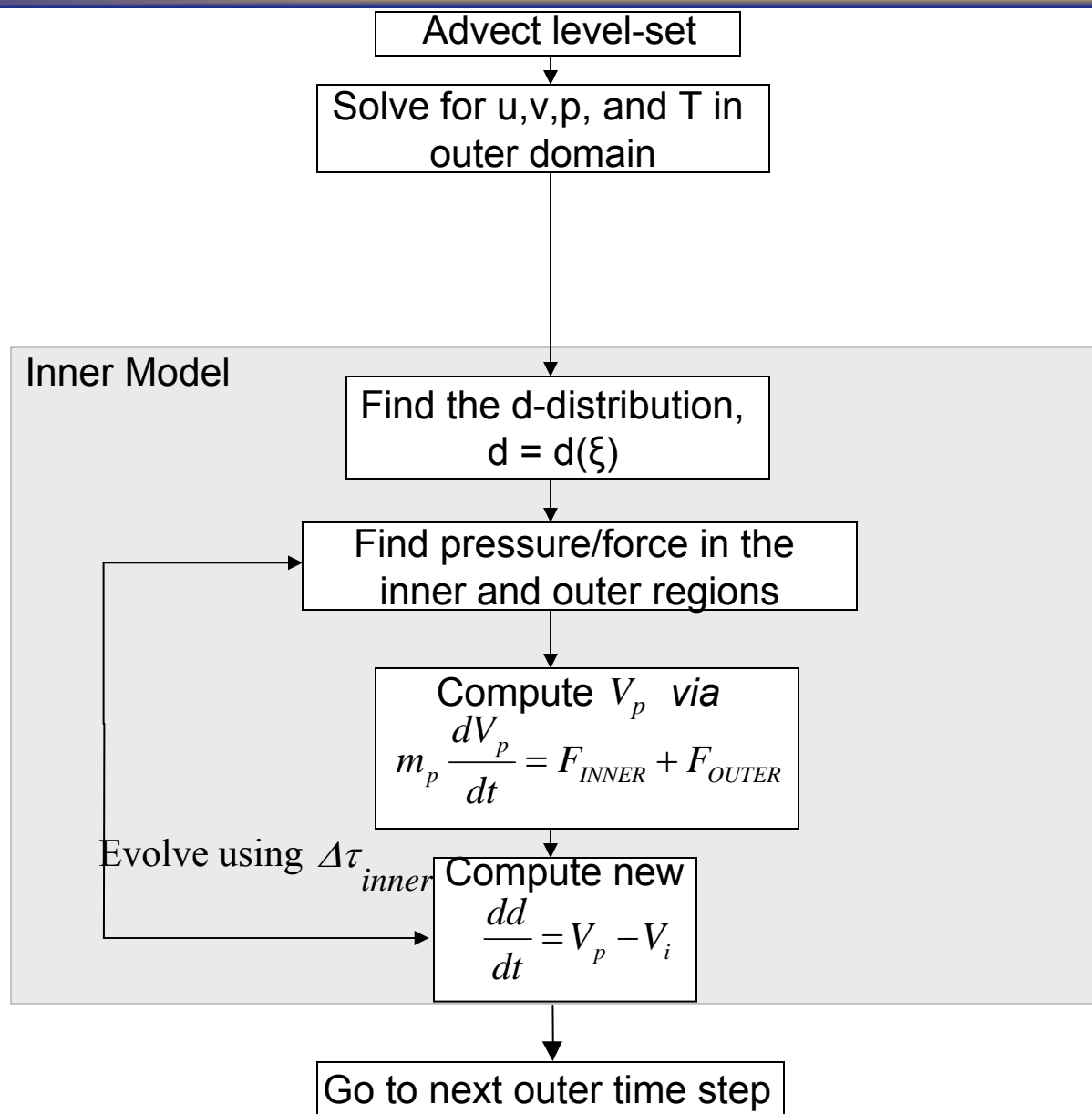
$$T_p = \left( \frac{q''}{k_l} \right) d + T_i$$







# Flowchart of calculation



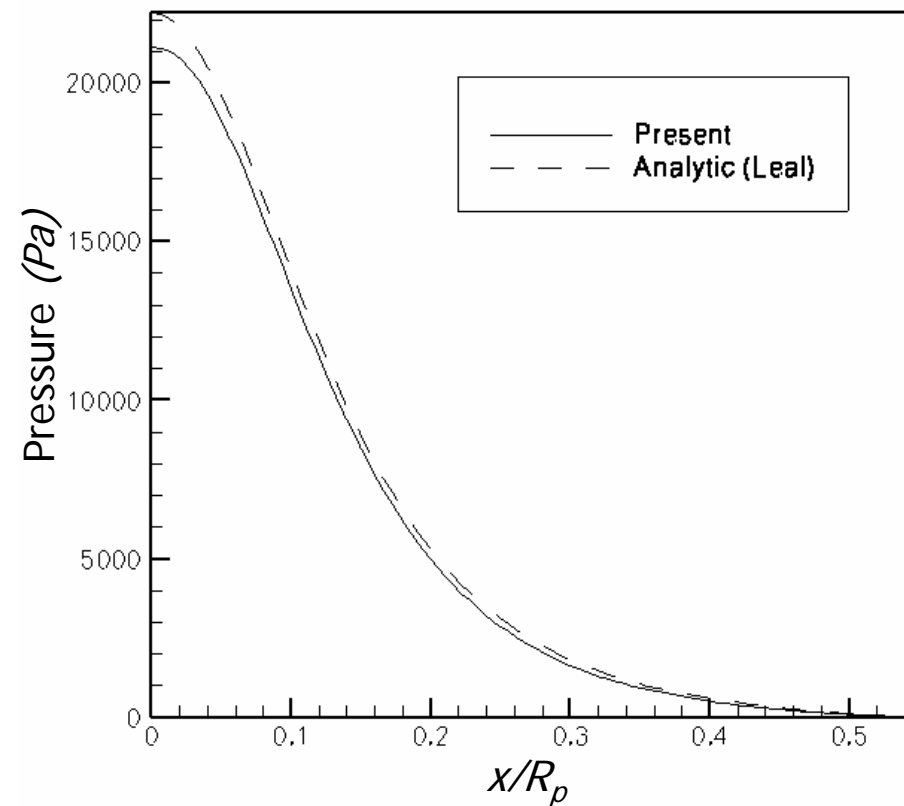
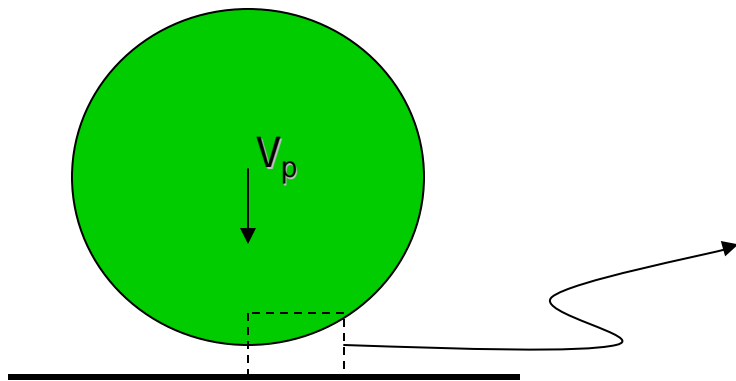


Results for particle+stable (non-dendritic)  
solidification front



## Validation of coupled model

- Compare model solution to an analytic solution for a simplified case
  - Particle approaching flat stationary interface (no disjoining pressure)<sup>1</sup>
- $d/R_p = 0.02$ , Particle velocity = 500 microns/sec,  $R_p = 1$  micron



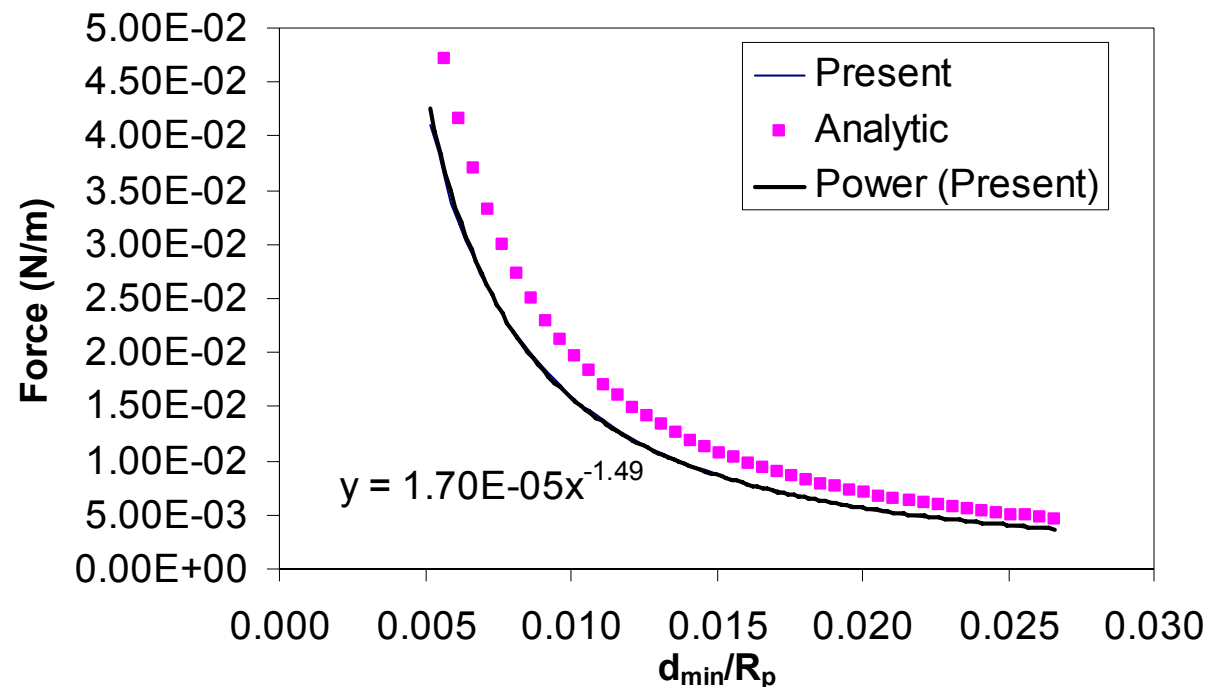
1. Gary L. Leal, Laminar flow and convective transport processes : scaling principles and asymptotic analysis (1992).



## Validation of coupled model

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F vs.  $d_{\min}/R_p$



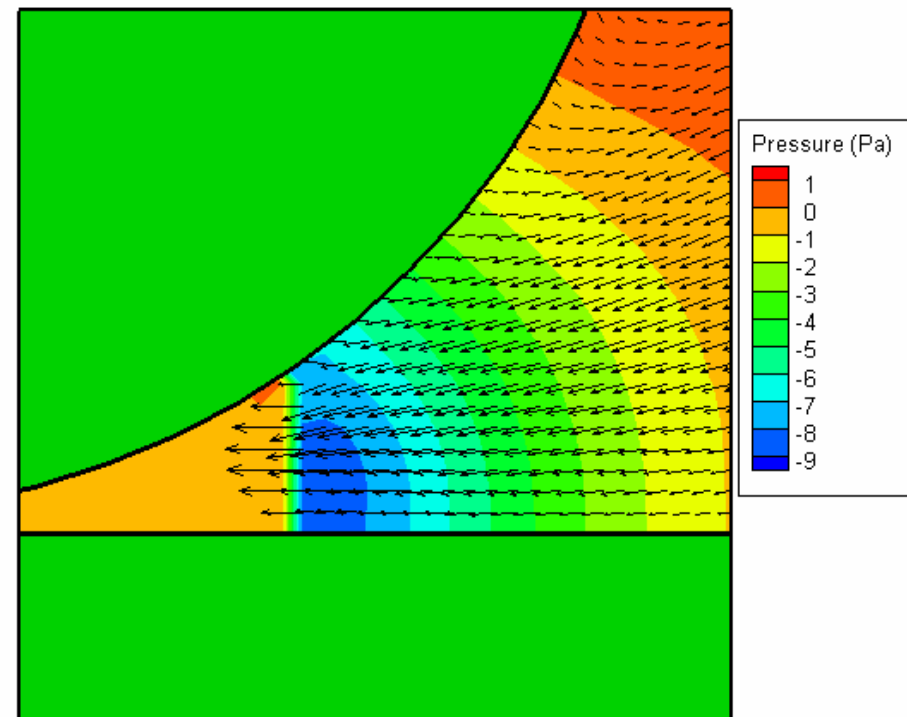
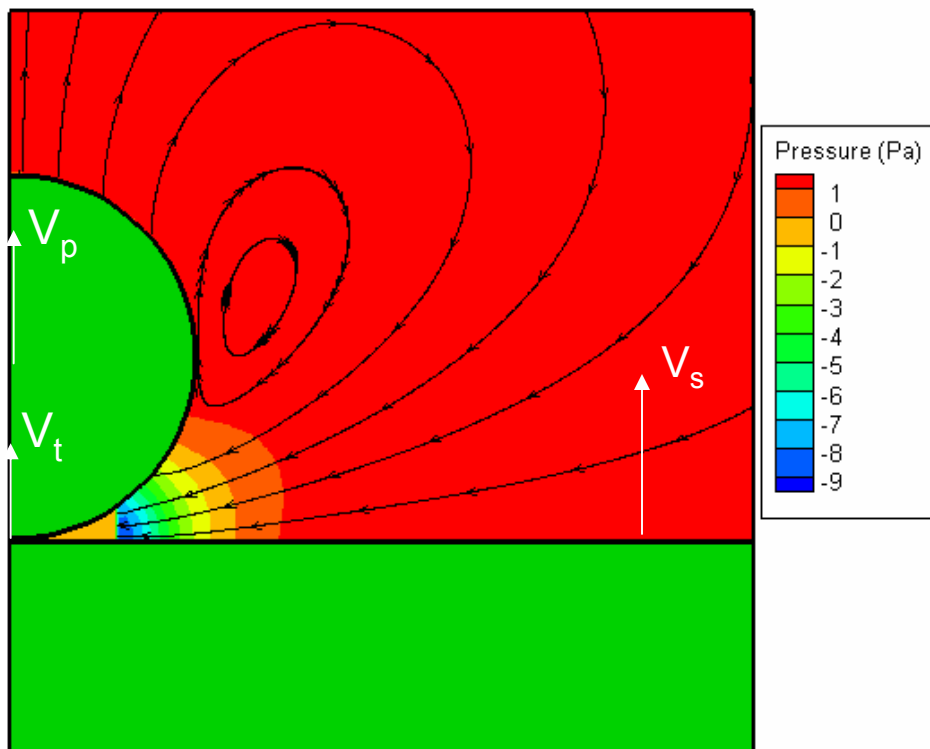
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## Planar Solidification front + particle



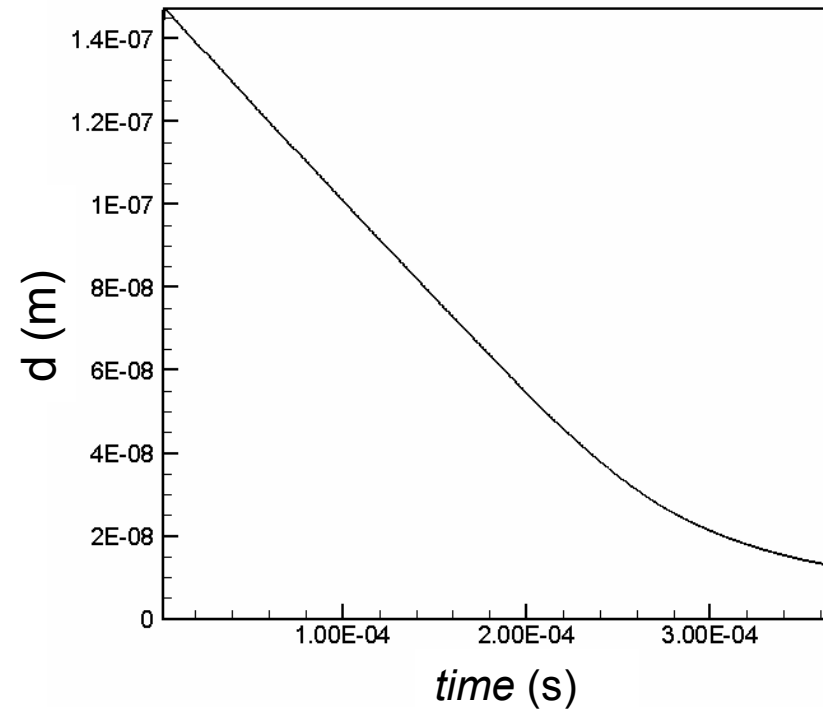
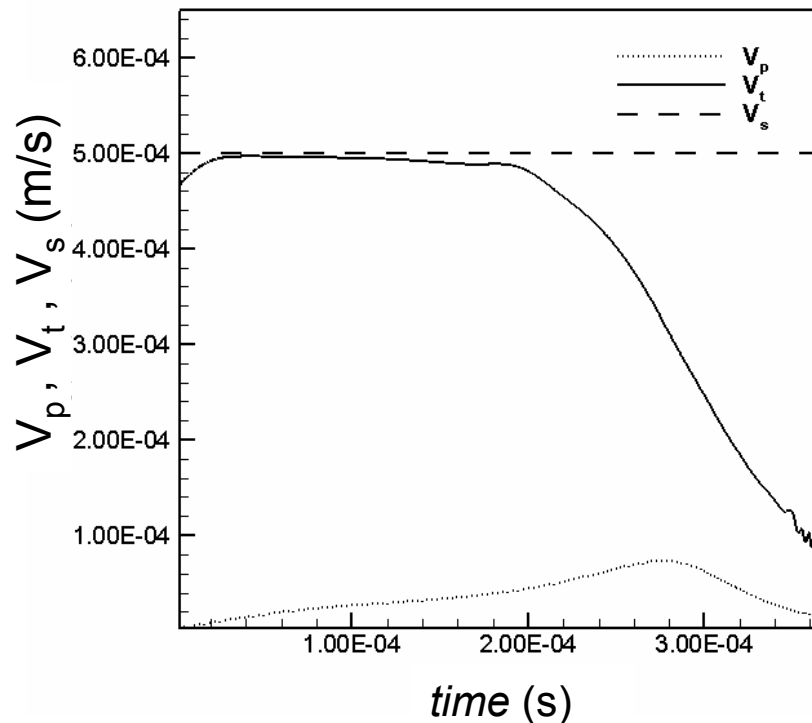
Solidification velocity = 500 microns/sec,  $R_p = 1$  micron, Hamaker =  $-8E-19$  J,  
 $k_p/k_l = 1.0$  (planar), no premelting





## Velocity vs. $t$ and $d$ vs. $t$ plots – premelting

Solidification velocity = 500 microns/sec,  $R_p = 1$  micron, Hamaker =  $-8E-19$  J,  
 $k_p/k_l = 1.0$  (planar), premelting

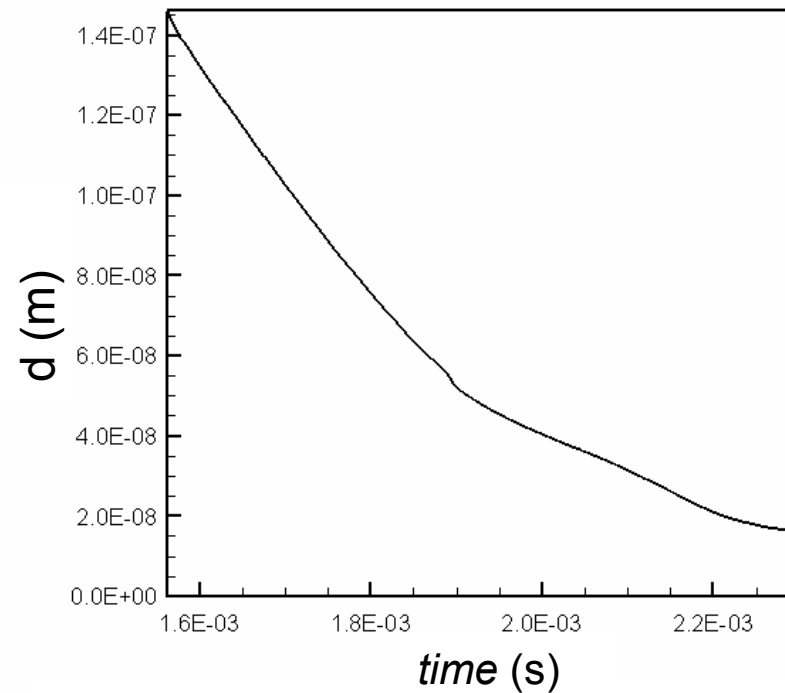
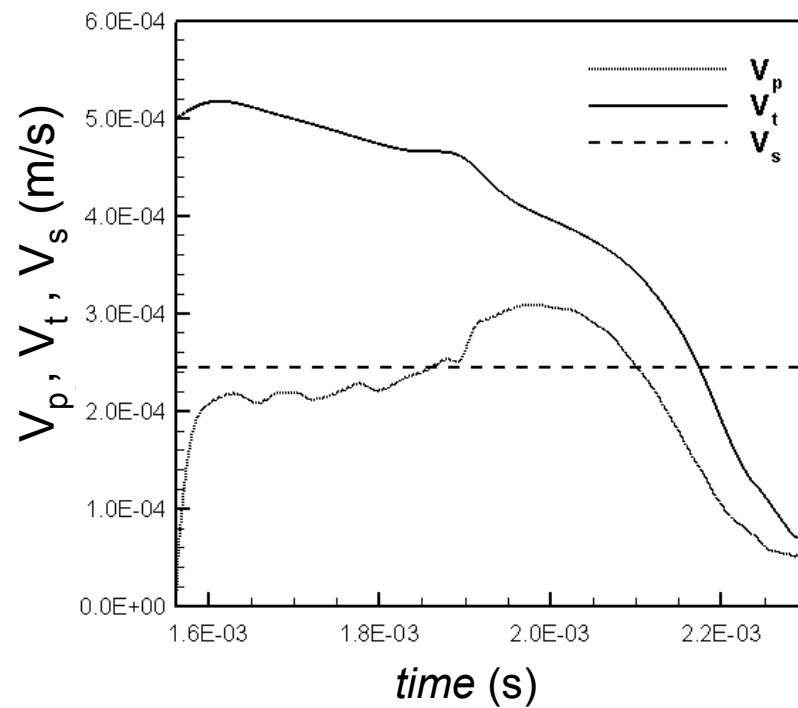


$k_p/k_l \geq 1.0$  ALWAYS ENGULFS!



## What about $k_p/k_l < 1.0$

Solidification velocity = 245 microns/sec,  $R_p = 1$  micron, Hamaker =  $-8E-19$  J,  
 $k_p/k_l = 0.01$ , premelting

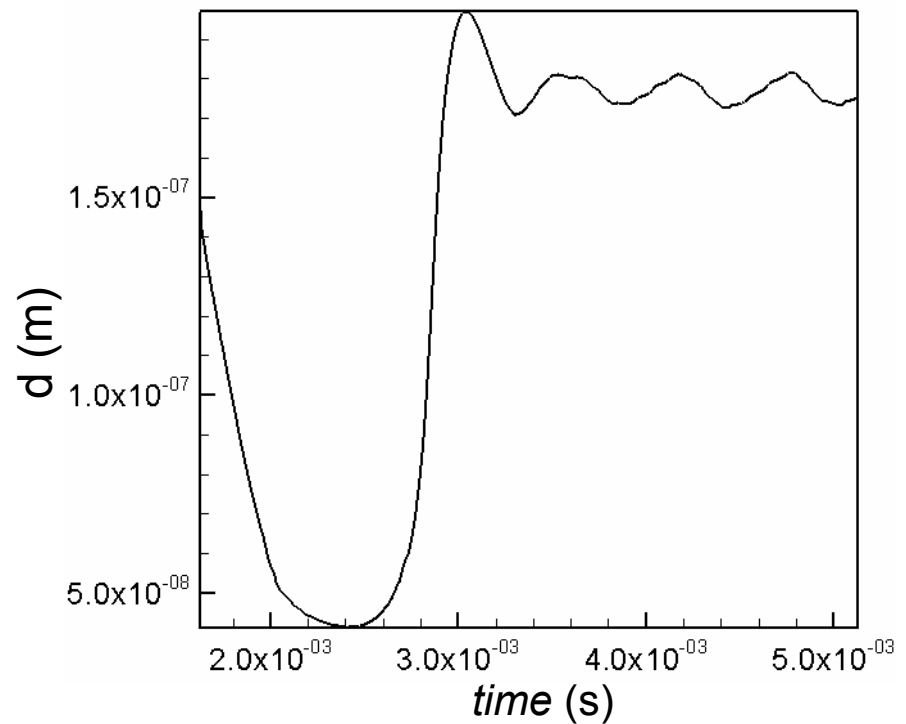
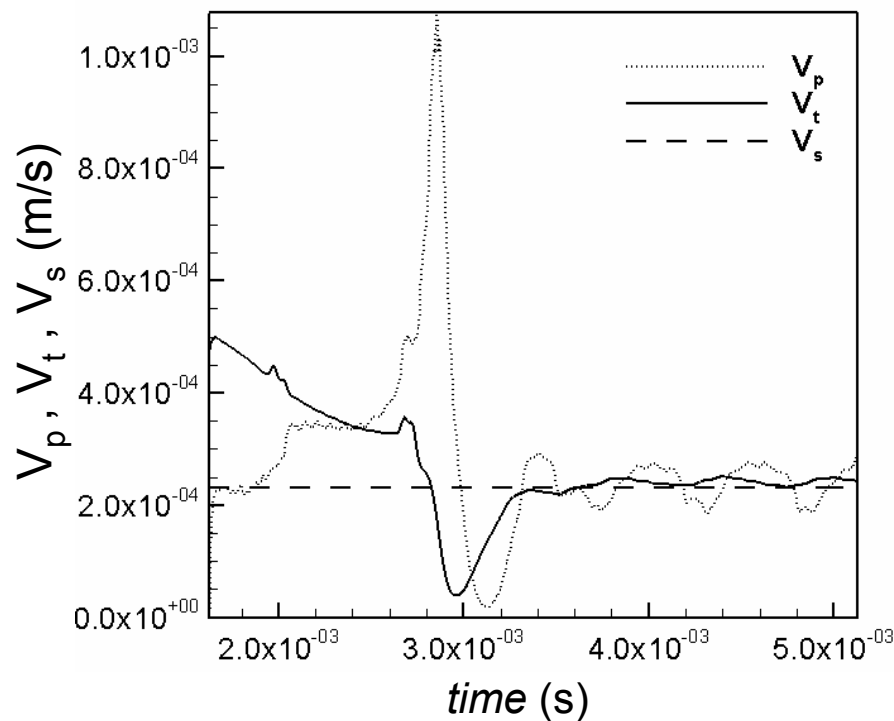


This one is engulfed!



## What about $k_p/k_l < 1.0$

Solidification velocity = 230 microns/sec,  $R_p = 1$  micron, Hamaker =  $-8E-19$  J,  
 $k_p/k_l = 0.01$ , premelting

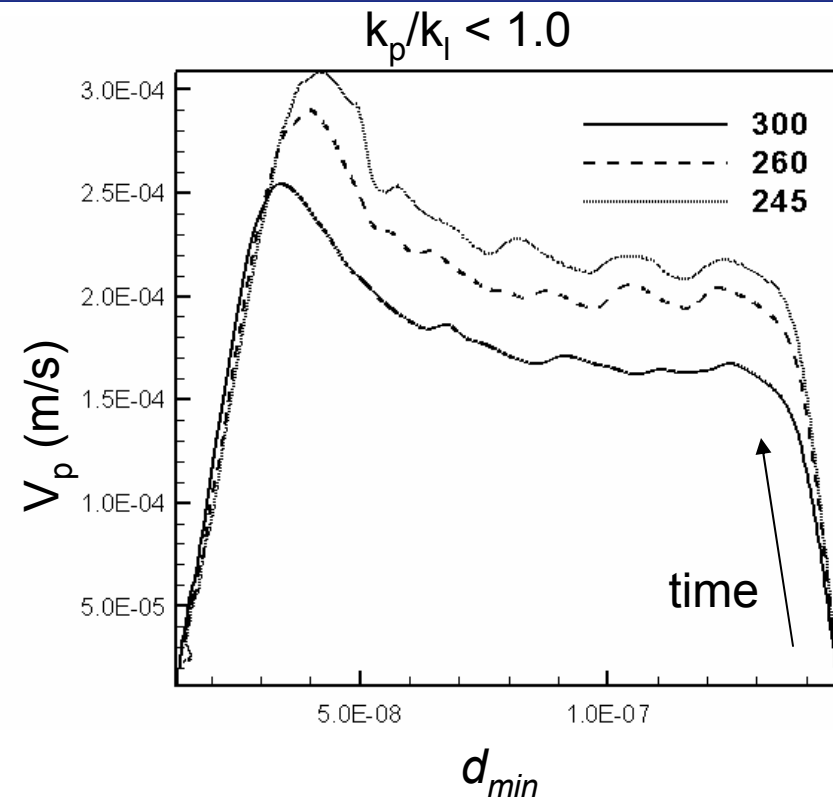
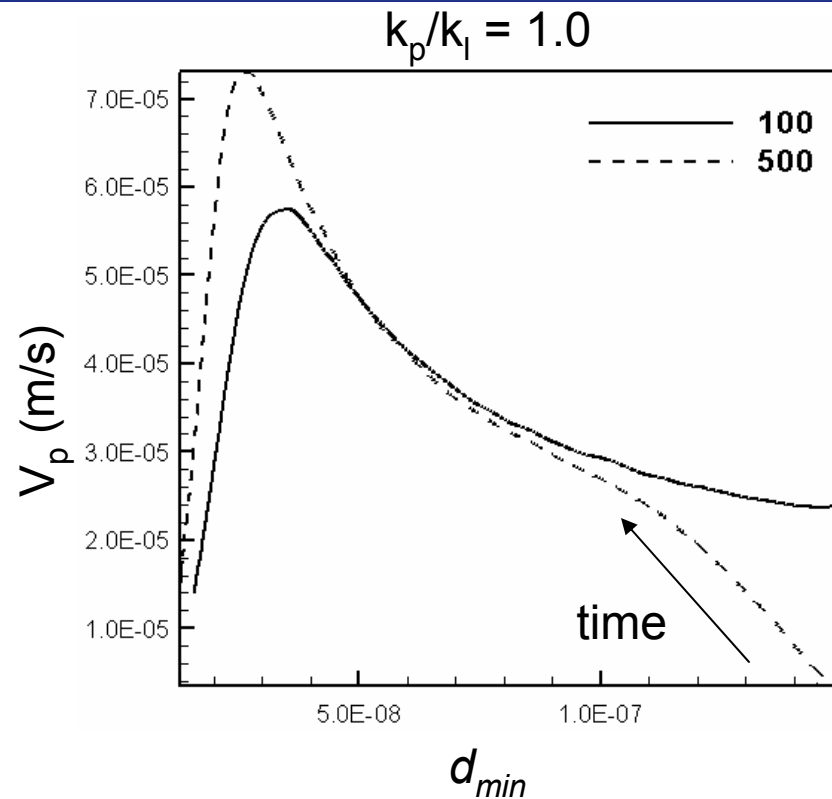


This one is Pushed!





## Phase-Space Plots -- engulfment

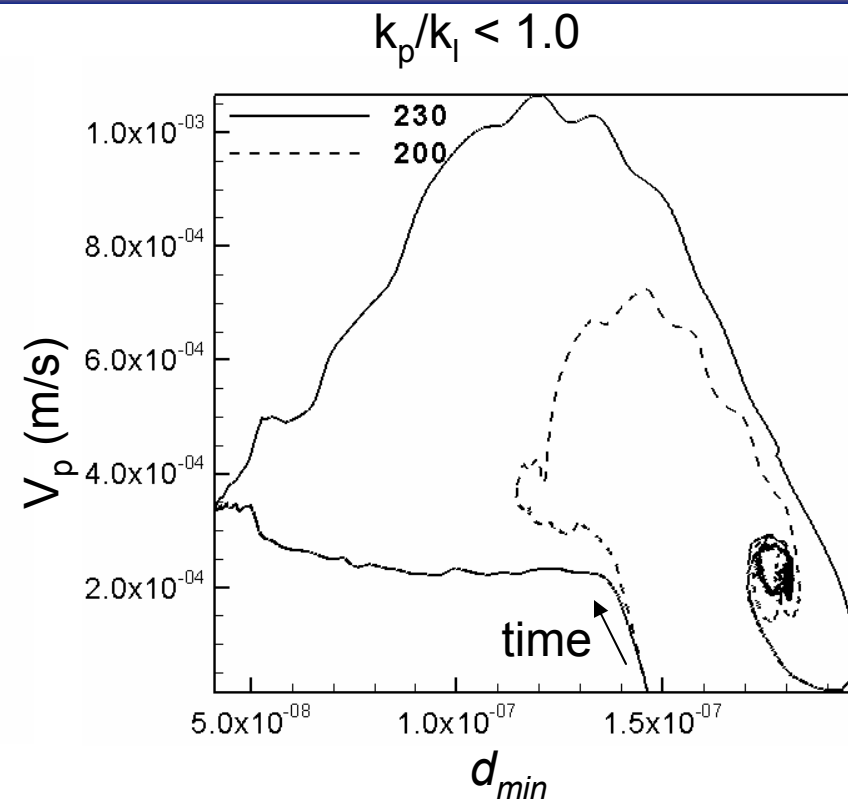
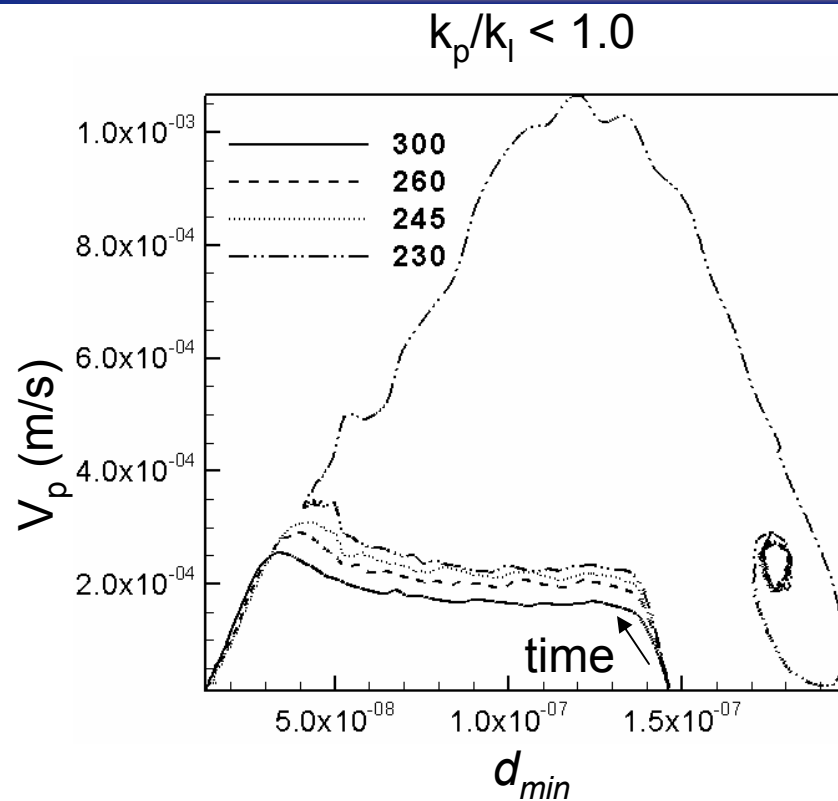


### NOTE:

- Similarity to Rempel and Worster – steady-state
- $k_p/k_l = 1.0 \rightarrow$  Rempel and Woster claim pushing at certain values, current claim is always engulfment



## Phase-Space Plots – engulfment/pushing



- 2 “attractors” in phase-space – engulfment/pushing
- Slightest change causes drastically different path to different region
- Reason: Interface never gets a chance to “bend”



## Conclusions of results section:

- 1) For  $k_p/k_l \geq 1$ , engulfment always occurs
- 2) For  $k_p/k_l < 1$ , the critical velocity can be found from dynamical considerations and occurs the moment the solidification front velocity is such that the particle “outruns” the tip velocity

## Main Contributions:

1. Developed a multiscale numerical approach to solve particle-solidification front problems in a general manner
2. Model captures essential physics that past research has neglected
3. First to look at the physics from a nonlinear dynamics point-of-view (i.e. phase-space point of view)
4. Model can be generalized to solve a variety of problems involving interacting interfaces



# Overall Conclusions

- A. Multiscale method was developed
  - 1. Capturing the interaction dynamics between two arbitrary solid objects
  - 2. Coupled two distinct regions (“inner” and “outer”) using a ‘matched numerics approach’
  
- B. Application of interest
  - 1. Particle-solidification front interactions
    - a. Engulfment occurs for  $k_p/k_l \geq 1$ .
    - b. For  $k_p/k_l < 1$ , the critical velocity is found using dynamical considerations
    - c. No assumptions are made as to the force equations or the way in which the critical velocity is obtained (i.e. no cut-off gap thickness value), etc...